AMENDMENTS TO THE CLAIMS

1. (Currently Amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

wherein the instance of chemical structural symmetry includes chemically symmetrically equivalent atoms and bonds;

determining an arrangement of the chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical structural symmetry in the chemical structure diagram;

laying out the chemically symmetrically equivalent atoms and bonds in the chemical structure diagram to visually express the identified symmetry in a stylized in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement; and

outputting the pictorial representation of the chemical structure.

2-8. (Canceled)

9. (Currently Amended) A computer-readable storage medium encoded with a set of instructions for use in a computer system to cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes symmetrically equivalent atoms and bonds;[[and]]

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determine an arrangement of the chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical structural symmetry in the chemical structure diagram;

lay out the chemically symmetrically equivalent atoms and bonds in the chemical structure diagram to visually express the identified symmetry in a stylized in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement; and

output the pictorial representation of the chemical structure.

10-12. (Canceled)

13. (Currently Amended) The method of claim 1, wherein the identified instance of chemical structural symmetry is based on rotational symmetry.

14. (Currently Amended) The method of claim 1, wherein the identified instance of chemical structural symmetry is based on reflective symmetry.

15. (Currently Amended) The method of claim 1, wherein the identified instance of chemical structural symmetry is based on inversive symmetry.

16. (Currently Amended) The method of claim 1, further comprising:

basing the identification of an instance of chemical structural symmetry on stereochemistry.

17. (Currently Amended) The method of claim 1, further comprising:

basing the identification of an instance of chemical structural symmetry on rotational symmetry, reflective symmetry, and stereochemistry.

18. (Currently Amended) The method of claim 1, further comprising:

basing the identification of an instance of chemical structural symmetry on double bond stereochemistry.

19. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

determining a pivot point for the instance of chemical structural symmetry[[list]].

20. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

determining a graph-theoretic center for the instance of chemical structural symmetry[[list]].

21. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

determining whether an atom belongs to the identified instance of chemical structural symmetry.

23. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

determining whether a bond belongs to the identified instance of chemical structural symmetry.

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24. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

in the event the identified instance of chemical structural symmetry is reflective, selecting a position for at least one of the chemically symmetrically equivalent atoms and bonds on an opposite side of a mirror line.

25. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

in the event the identified instance of chemical structural symmetry is rotative, selecting a position for at least one of the chemically symmetrically equivalent atoms and bonds based on a pivot point.

26. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. (Currently Amended) The method of claim 1, the determining an arrangement of the chemically symmetrically equivalent atoms and bonds further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.

28. (Currently Amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying an instance of chemical structural symmetry in the chemical structure;

wherein the instance of <u>chemical structural</u> symmetry includes symmetrically equivalent atoms and bonds;

<u>determining an arrangement of the chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical symmetry in the chemical structure diagram;</u>

laying out <u>the chemically</u> symmetrically equivalent atoms and bonds in the chemical structure diagram ~~to visually express the identified symmetry in a stylized~~ <u>in a</u> two-dimensional pictorial representation of the chemical structure <u>in accordance with the determined arrangement</u>; and

outputting the pictorial representation of the chemical structure.

29. (Currently Amended) The method of claim 28, wherein the <u>identified</u> instance of chemical structural symmetry is based on rotational symmetry.

30. (Currently Amended) The method of claim 28, wherein the <u>identified</u> instance of chemical structural symmetry is based on reflective symmetry.

31. (Currently Amended) The method of claim 28, wherein the <u>identified</u> instance of chemical structural symmetry is based on inversive symmetry.

32. (Currently Amended) The method of claim 28, further comprising:

basing the identification <u>of an instance of chemical structural symmetry</u> on stereochemistry.

33. (Currently Amended) The method of claim 28, further comprising:

basing the identification <u>of an instance of chemical structural symmetry</u> on rotational symmetry, reflective symmetry, and stereochemistry.

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34. (Currently Amended) The method of claim 28, further comprising:

basing the identification of an instance of chemical structural symmetry on double bond stereochemistry.

35. (Currently Amended) A computer-readable storage medium encoded with a set of instructions to cause a system to derive a chemical structure diagram, the instructions causing the system to:

identify an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes chemically symmetrically equivalent atoms and bonds;

determine an arrangement of the chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical symmetry in the chemical structure diagram;

lay out the chemically symmetrically equivalent atoms and bonds in the chemical structure diagram to visually express the identified symmetry in a stylized in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement; and

output the pictorial representation of the chemical structure.

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